OLCI Level 2

Algorithm Theoretical Basis Document

Ocean Colour Products in Case 1 waters

("Clear Waters Ocean Colour Products" or "CWOC")

DOCUMENT REF: Deliverable Ref: S3-L2-SD-03-C10-LOV-ATBD SD-03-C

VERSION:

2.3

OLCI Level 2 Algorithm Theoretical Basis Document Ocean Colour Products in case 1 waters

Document Signature Table

	Name	Function	Company	Signature	Date
Prepared	D. Antoine	OLCI Expert	Consultant	Jule	5 October 2012
	O. Fanton d'Andon	OLCI coordinator	ACRI-ST		
Approved	L. Bourg	OLCI expert	ACRI-ST		
Released	O. Fanton d'Andon	OLCI coordinator	ACRI-ST		

Change record

Issue	Date	Description	Change pages
2.0	March 30, 2010	Version 2 for CDR delivery	
2.1	April 10, 2010	Minor Updates	
2.2	July 13, 2010	Version 2.2 for CDR delivery	Clarified list of products in Section 3.3.1
2.3	5 October 2012	Version 2.3 for final delivery	Section on uncertainty has been added (3.2.2)

Distribution List

Organisation	То
ESA	Philippe Goryl, Alessandra Buongiorno and Carla Santella
EUMETSAT	Vincent Fournier-Sicre and Vincenzo Santacesaria
CONSORTIUM PARTNERS	ARGANS, ACRI-ST, RAL, Brockmann Consult, Elsag-Datamat

Table of content

1. INTRODUCTION	6
1.1 Purpose and scope	6
1.2 Acronyms	6
1.3 Symbols	7
1.4 Algorithm identification	8
2. ALGORITHM OVERVIEW	9
2.1 Objectives	9
3. ALGORITHM DESCRIPTION	10
3.1 Theoretical Description	10
3.1.1 The chlorophyll concentration, Chl	10
3.1.2 The diffuse attenuation coefficient at 490 nm, $K_d(490)$	
3.1.3 The total absorption and backscattering coefficients (a and bb)	
3.1.4 Can the CDOM absorption coefficient (ag) be derivable?	
3.1.5 Alternative approach: the GSM algorithm	
3.2 Error estimates	
3.2.1 Semi-empirical algorithm	23
3.2.2 GSM algorithm	24
3.3 SUMMARY OF RECOMMENDATIONS	
3.3.1 Products	
3.3.2 Pixel-by-pixel error estimates	
4. ASSUMPTIONS AND LIMITATIONS	
4.1 Assumptions	
4.2 Constraints, limitations	
5. REFERENCES	29
6. APPENDIX: BBW COMPUTATION	

List of Figures

Figure 1: Adapted from Fig. 6 of Morel 2007: Ratios $\rho_{2,5}$, $\rho_{3,5}$, $\rho_{4,5}$ of reflectances at 443, 490, and 510 nm (indices 2, 3, and 4) to the reflectance at 560 nm (indice 5), as a function of the Chlorophyll concentration. The corresponding algorithms making use of only 2 wavelengths are denoted OC2Me-443, OC2Me-490, and OC2Me-510. The envelope of these three curves (maximum band ratio technique) forms the currently used MERIS algorithm, denoted OC4Me. The ρ is the log₁₀ of the Figure 2: Adapted from Fig. 7 of Morel 2007: "The maximum band ratio technique, represented by the curve reproduced from Fig. 6, is compared to recent measurements of irradiance reflectance, made at sea during the following cruises: Bencal (Benguela current, 2002), Biosope, (South-East Figure 3: reproduced from Morel et al. (2007a): validation of the OK2-555 algorithm against the NOMAD in situ data set (Werdell and Bailey, 2005).....13 Figure 4: Validation of the proposed IOP algorithm against the synthetic data set of IOCCG (IOCCG, 2006). The four panels are for total absorption and total backscattering at two wavelengths. The parameters of a linear regression on the log-transformed data are provided in each panel. Here K_d and R are taken from the synthetic data set so they are independent Figure 5: Validation of the proposed IOP algorithm against the *in situ* data set of IOCCG (IOCCG, 2006). The four panels are for total absorption at four wavelengths (no backscattering measurements in the IOCCG data set). Here, Kd has been derived from Chl before entering into the algorithm (no K_d data within the IOCCG in situ data base). The parameters of a linear regression on the log-transformed data are provided in each panel. Note: data from the Chesapeake bay and its vicinity (experiment name: "LMER-TIES"), suspected of having been collected in Case 2 waters, have been removed from the data hase

Figure 6: Validation of the proposed algorithm for the particulate backscattering coefficient, against *in situ* data from the BOUSSOLE site (Antoine et al., 2006; hydroscat-II instrument), the Plumes and Blooms site (Kostadinov et al., 2007; hydroscat-VI instrument), and the NOMAD v2 data set (Werdell and Bailey, 2005; various instrument). The parameters of a linear regression on the log-transformed data are provided. The shaded area corresponds to

Figure 9: example of error calculation following Eq. (19). The errors are given on the figure.

1. INTRODUCTION

1.1 Purpose and scope

This Algorithm Theoretical Basis document (ATBD) is written for the Ocean and Land Colour Imager (OLCI) of the Earth Observation Mission Sentinel-3 of the European Space Agency (ESA).

The purpose of this document is to lay out algorithms for the OLCI ocean colour products in Case 1 waters. As much as possible, basic principles of the algorithm and the description of their various segments will refer to publications in the peer-reviewed scientific literature. When such literature exists, minimum information will be provided here for the sake of clarity, and the reader will be referred to the relevant literature for further information.

1.2 Acronyms

ATBD	Algorithm Theoretical Basis Document
CDOM	Colored Dissolved Organic Matter
ENVISAT	Environmental Satellite
ESA	European Space Agency
LOV	Laboratoire d'Océanographie de Villefranche
MERIS	Medium Resolution Imaging Spectrometer
NASA	National Aeronautics & Space Administration
nLw	Normalized Water-leaving radiance
NOMAD	NASA bio-Optical Marine Algorithm Data set
OC	Ocean Color
OLCI	Ocean and Land Color Imager
PnB	Plumes and Blooms (Bio-optics time series in the Santa Barbara Channel)
SeaWiFS	Sea-viewing Wide Field-of-view Sensor
Sentinel-3	Third series of "sentinel" (ESA satellites)
ТОА	Top of Atmosphere
UV	Ultra Violet

1.3 Symbols

Symbol	definition	Dimension / units
Constant	and a subsec	
Geometry, wavel	engths, others	
λ	Wavelength $S_{\rm eff} = cos(0)$	nm
<i>U</i> s	Sun zenitn angle ($\mu_s = \cos(\theta_s)$)	degrees
Øv Ad	Satellite viewing angle ($\mu v = \cos(\theta v)$)	degrees
$\Delta \varphi$	half vertical planes	degrees
Chl	Chlorophyll concentration	mg m ⁻³
Radiometry and A	Apparent Optical properties (AOPs)	
$F_0(\lambda)$	Mean extraterrestrial spectral irradiance	$W m^{-2} nm^{-1}$
$L(\lambda, \theta_s, \theta_v, \Delta \phi)$	Radiance	$W m^{-2} nm^{-1} sr^{-1}$
E _d (z)	Downward irradiance at depth z	W m ⁻² nm ⁻¹
E _u (z)	Upward irradiance at depth z	W m ⁻² nm ⁻¹
$E_{d}(0^{+})$	Downward irradiance just above the sea surface	W m ⁻² nm ⁻¹
R(λ, 0 ⁻)	Diffuse reflectance at null depth, or irradiance ratio (E_u / E_d)	dimensionless
	(upward and downward irradiances, respectively)	
$K_d(\lambda)$	Diffuse attenuation coefficient for the downward plane	m^{-1}
	irradiance	
$K_{W}(\lambda)$	Contribution of seawater to $\mathrm{K}_{\mathrm{d}}(\lambda)$	m ⁻¹
f	Ratio of $R(0)$ to (b_b/a) ; subscript 0 when $\theta_s = 0$	dimensionless
f	Ratio of R(0 ⁻) to ($b_b/(a+b_b)$); subscript 0 when $\theta_s = 0$	dimensionless
μ_d	Average cosine of the downward irradiance	dimensionless
$Q(\lambda, \theta s, \theta v, \Delta \phi)$	Factor describing the bidirectional character of $R(\lambda, 0)$ Q = E_u / L_u . Subscript 0 when $\theta_s = \theta_v = 0$,	sr
$ ho_{ m w}(\lambda)$	Water-leaving reflectance (<i>i.e.</i> , π L _w / E _d (0 ⁺))	dimensionless
$[ho_{ m W}]_{ m N}(\lambda)$	Normalised water-leaving reflectance (<i>i.e.,</i> the reflectance if	
	there were no atmosphere, and for $\theta_{\rm S} = \theta_{\rm V} = 0$)	

dimensionless

Inherent optical properties (IOPs)

$a(\lambda)$	Total absorption coefficient	m^{-1}
$a_w(\lambda)$	Water absorption coefficient	m ⁻¹
$a_{\mathrm{ph}}(\lambda)$ or $a_{\mathrm{f}}(\lambda)$	Phytoplankton absorption coefficient	m ⁻¹
$a_{g}(\lambda)$ or $a_{cdom}(\lambda)$	CDOM absorption coefficient	m ⁻¹

		Ref: S3-L2-SD-03- C10-LOV-ATBD
David ANTOINE	SENTINEL-3 OPTICAL PRODUCTS AND ALGORITHM	Issue: 2.3
Daria	DEFINITION	Date: 5 October 2012
	OLCI Level 2 Algorithm Theoretical Basis Document	Page:8
	Ocean Colour Products in case 1 waters	

$a_{cdm}(\lambda)$	Coloured detrital material absorption coefficient	m^{-1}
$b_b(\lambda)$	Total backscattering coefficient	m ⁻¹
$b_{bw}(\lambda)$	Water backscattering coefficient	m ⁻¹
$b_{bp}(\lambda)$	Particulate backscattering coefficient	m ⁻¹

Air-water interface

 $\Re(\theta)$ Geometrical factor, accounting for all refraction and reflection dimensionless effects at the air-sea interface (Morel and Gentili, 1996)

$$\Re(\theta') = \left[\frac{(1-\overline{\rho})}{(1-\overline{r}R)} \frac{(1-\rho_{\rm F}(\theta'))}{n^2}\right] (\text{subscript } 0 \text{ when } \theta' = 0)$$

	where n is the refractive index of water	dimensionless
	$ ho_{ m F}(heta)$ is the Fresnel reflection coefficient for incident angle $ heta$	dimensionless
	$\overline{ ho}$ is the mean reflection coefficient for the downward	dimensionless
	irradiance at the sea surface	
	\tilde{r} is the average reflection for upwelling irradiance at the water-air interface	dimensionless
	θ' is the refracted viewing angle ($\theta' = \sin^{-1}(n.\sin(\theta_v))$)	degrees
Others		
$t_d(\lambda, \theta_s)$	Upward diffuse atmospheric transmittance (pixel-to-sensor)	dimensionless
$t_{s}(\lambda, \theta_{s})$	Downward global atmospheric transmittance (E_d(0 ⁺) / F_0 $\mu_{s})$	dimensionless

1.4 Algorithm identification

This algorithm is identified under reference "SD-03-C10" in the Sentinel-3 OLCI documentation.

In this document, it will be referred to as "CWOC", standing for "Clear-Water Ocean Colour Products".

2. ALGORITHM OVERVIEW

2.1 Objectives

The objective is to derive several ocean colour products from the spectrum of the normalised water-leaving reflectances.

The following products are to be derived here:

- The chlorophyll concentration, Chl, expressed in units of mg (Chl) m⁻³.
- The diffuse attenuation coefficient for downward irradiance at 490 nm, K_d(490), expressed in units of m⁻¹.
- The total absorption and backscattering coefficients, a and b_b, expressed in units of m⁻¹.
- The CDOM absorption coefficient, expressed in units of m⁻¹.

The proposed algorithms are from Morel et al. (2006; 2007a) (see also the latest version of the MERIS ATBD 2.9 for the chlorophyll concentration), and from Maritorena et al. (2002).

Note: the products presented here are all derived from various combinations of the fully normalized water-leaving reflectances. The latter are actually the main ocean colour product above Case 1 waters. There is no need to describe them in this document, however; they are simply the output of the atmospheric correction algorithm, for which a specific ATBD exists [SD-03-CO7].

3. ALGORITHM DESCRIPTION

3.1 Theoretical Description

3.1.1 The chlorophyll concentration, Chl

The proposed algorithm is the "OC4Me" maximum-band-ratio (MBR) semi-analytical algorithm developed by Morel et al. (2007a). (*cf.* O'Reilly *et al.*, 1998 for a more general description of such algorithms)

It is the latest version of the MERIS pigment index algorithm, which is fully described in the MERIS ATBD 2.9¹ and in Morel et al. (2007a). A brief reminder is provided here:

OC4Me is a polynomial based on the use of a semi-analytical model, itself based on the analysis of AOPs measured *in situ* over the past decades in various oceanic regions (Morel 1988; Morel and Maritorena, 2001).

It is expressed as:

$$\log_{10} [Chl] = \sum_{x=0}^{n} A_{x} (\log_{10} [\rho_{i,j}])^{x}$$
(1)

where $\rho_{i,j}$ is the ratio of the irradiance reflectance, R, at band i (λ_i) to the irradiance reflectance at band j (λ_j). The value of this ratio is the maximum found among the 3 ratios formed with the following bands: 560 nm for λ_j , and 443 or 490 or 510 nm for λ_i . In Eq. (1), n is equal to 4.

Figures 1 and 2 show how the algorithm behaves.

The "A" coefficients to be used are (Morel et al., 2007a):

	- 4
0.4502748 -3.259491 3.522731 -3.359422	0.949586

Table 1. Coefficients in Eq. (1)

Because this algorithm uses R and the MERIS atmospheric correction provides directional reflectances, ρ_{w} , a conversion is needed as follows:

$$R = \frac{\rho_w Q}{\pi \Re}$$
(2)

The Q factor is from Morel et al., 2002 (it is chlorophyll-dependent so an iterative procedure is needed similarly as in Morel and Gentili, 1996).

¹ Latest version available at <u>http://envisat.esa.int/instruments/meris/pdf/</u>

		Ref: S3-L2-SD-03- C10-LOV-ATBD
David ANTOINF	SENTINEL-3 OPTICAL PRODUCTS AND ALGORITHM	Issue: 2.3
	DEFINITION	Date: 5 October 2012
	OLCI Level 2 Algorithm Theoretical Basis Document	Page:11
	Ocean Colour Products in case 1 waters	

The \Re geometrical factor merges all reflection / refraction effects at the air-sea interface. It is defined as (Morel and Gentili, 1996):

$$\Re(\theta') = \left[\frac{(1-\bar{\rho})}{(1-\bar{r}R)} \frac{(1-\rho_{\rm F}(\theta'))}{n^2}\right] \text{ (subscript 0 when } \theta'=0)$$
(3)

where

n is the refractive index of water

 $\rho F(\theta)$ is the Fresnel reflection coefficient for incident angle θ

 $\overline{\rho}$ is the mean reflection coefficient for the downward irradiance at the sea surface

 $\tilde{\mathbf{r}}$ is the average reflection for upward irradiance at the water-air interface

 θ is the refracted viewing angle (θ = sin⁻¹(n sin(θ v)))

In Eq. (3), the dependence of $\overline{\rho}$ and R on θ_s are neglected. This dependence was recently shown significant for low sun elevations by Wang (2006). It is here proposed to include this effect, which can be done easily by adding one more dimension to the R lookup tables currently in use.



Figure 1: Adapted from Fig. 6 of Morel 2007: Ratios Figure 2: Adapted from Fig. 7 of Morel 2007: "The $\rho_{2.5}$, $\rho_{3.5}$, $\rho_{4.5}$ of reflectances at 443, 490, and 510 nm maximum band ratio technique, represented by the (indices 2, 3, and 4) to the reflectance at 560 nm (indice curve reproduced from Fig. 6, is compared to recent 5), as a function of the Chlorophyll concentration. The measurements of irradiance reflectance, made at sea corresponding algorithms making use of only 2 during the following cruises: Bencal (Benguela current, wavelengths are denoted OC2Me-443, OC2Me-490, and 2002), Biosope, (South-East Pacific, 2004), Aopex, OC2Me-510. The envelope of these three curves (Western Mediterranean Sea, 2004)." (maximum band ratio technique) forms the currently used MERIS algorithm, denoted OC4Me. The ρ is the log10 of the maximum of the 3 ($\rho_{2,5}$, $\rho_{3,5}$, $\rho_{4,5}$) ratios

Recommendation: use the OC4Me algorithm, and include a θ_s -dependence in the \Re lookup table.

		Ref: S3-L2-SD-03- C10-LOV-ATBD
David ANTOINE	SENTINEL-3 OPTICAL PRODUCTS AND ALGORITHM	Issue: 2.3
	DEFINITION	Date: 5 October 2012
	OLCI Level 2 Algorithm Theoretical Basis Document	Page:12
	Ocean Colour Products in case 1 waters	

3.1.2 The diffuse attenuation coefficient at 490 nm, $K_d(490)$

The diffuse attenuation coefficient for the downward plane irradiance at wavelength λ and at a given depth z is defined as:

$$K_d(\lambda) = - \left[\frac{1}{E_d(z, \lambda)} \right] \left[\frac{dE_d(z, \lambda)}{dz} \right] \text{ or } K_d(\lambda) = - \frac{d\left[\ln E_d(z, \lambda) \right]}{dz}$$
(3)

Many realisations of this coefficient are possible, as a function of the depth range over which it is computed. It can be a local coefficient around a given small depth interval between any depths z_1 and z_2 :

$$K_d(\lambda) = -\frac{\log[E_d(z_1, \lambda) / E_d(z_2, \lambda)]}{z_2 - z_1}$$
(5)

It can be computed for the upper layer defined from below the surface (0⁻) to a given depth *z*:

$$K_{d} = -\frac{\log \left[E_{d}(z) / E_{d}(0^{-}) \right]}{z}$$
(6)

It can also be an E_d-weighted average value computed over a certain depth *z*, e.g., the 1% light level (Kirk, 2003):

$$K_{d,av}(\lambda) = \frac{\int_{0}^{z} K_{d}(z,\lambda) E_{d}(z,\lambda) dz}{\int_{0}^{z} E_{d}(z,\lambda) dz}$$
(7)

Practically speaking, the K_d's found in *in situ* data bases are essentially of the second category. The reason is simply that measuring properly $E_d(z)$ at sea requires that the irradiance sensor is placed at a depth where the irradiance fluctuations due to surface waves are small enough (or even absent). This depth can be as large as ~30 meters in clear waters. Then this $E_d(z)$ measurement is combined with the downward irradiance measured above the surface after it is multiplied by the transmission across the air-sea interface, which provides $E_d(0^-)$, in order to get K_d as per Eq (6) above.

It is proposed here to use the "OK2-560" algorithm proposed by Morel et al. (2007a). It is based on the 490-560 reflectance ratio (see Fig. 3) and has the form:

$$K_{d}(490) = K_{w}(490) + 10^{\sum_{x=0}^{n} A_{x}(\log_{10} \rho_{490,560})^{x}}$$
(8)

where $K_w(490)$ is 0.0166 m⁻¹, $\rho_{490,560}$ is the ratio of the irradiance reflectances at 490 and 560 nm, and the n+1=5 coefficients A_x have the values :

		Ref: S3-L2-SD-03- C10-LOV-ATBD
David ANTOINE	SENTINEL-3 OPTICAL PRODUCTS AND ALGORITHM	Issue: 2.3
	DEFINITION	Date: 5 October 2012
	OLCI Level 2 Algorithm Theoretical Basis Document	Page:13
	Ocean Colour Products in case 1 waters	

A ₀	A ₁	A ₂	A ₃	A_4
-0,82789	-1,64219	0,90261	-1,62685	0,088504

Table 2. Coefficients to be used in Eq. (8)

Conversion from directional reflectances to irradiance reflectances is as per Eq. (2).

Recommendation: use the OK2-560 algorithm to determine $K_d(490)$.



Figure 3: reproduced from Morel et al. (2007a): validation of the OK2-555 algorithm against the NOMAD in situ data set (Werdell and Bailey, 2005)

3.1.3 The total absorption and backscattering coefficients (a and bb)

Many algorithms have been proposed to derive inherent optical properties (IOPs), particularly the total absorption coefficient (a_t) and the total backscattering coefficients (b_b) , from various AOPs (very often from R_{rs} or from R and K_d). It is out of scope here to enter into these details, and the reader is referred to the comprehensive review by Gordon (2002) and to IOCCG report N°5 (IOCCG, 2006).

In particular, the results of the inter-comparison presented in the IOCCG report don't reveal one algorithm as performing significantly better than the others (whatever their degree of complexity).

Therefore, it is proposed here to use a simple approach, as proposed by Morel et al. (2006); see their Eq. (10) to (13). This approach combines two equations (Gordon, 1989; Gordon et al., 1975; Morel and Gentili, 2004):

$$K_{d}(\lambda) = 1.0395 \left[a(\lambda) + b_{b}(\lambda)\right] / \mu_{d}$$
(9)

and

$$R(\lambda) = f' b_b(\lambda) / [a(\lambda) + b_b(\lambda)]$$
(10)

		Ref: S3-L2-SD-03- C10-LOV-ATBD
David ANTOINE	SENTINEL-3 OPTICAL PRODUCTS AND ALGORITHM	Issue: 2.3
	DEFINITION	Date: 5 October 2012
	OLCI Level 2 Algorithm Theoretical Basis Document	Page:14
	Ocean Colour Products in case 1 waters	

which leads to

$$a(\lambda) = 0.962 \text{ K}_{d}(\lambda) \mu_{d}(\lambda, \theta_{s'} \text{ Chl}) \times [1 - R(\lambda) / f'(\lambda, \theta_{s'} \text{ Chl})]$$
(11)

$$b_{b}(\lambda) = 0.962 \text{ K}_{d}(\lambda) \mu_{d}(\lambda, \theta_{s'} \text{ Chl}) \times [R(\lambda) / f'(\lambda, \theta_{s'} \text{ Chl})]$$
(12)

where the dependence of f' and μd on the sun zenith angle and Chl is explicitly introduced. These two parameters are taken from pre-computed lookup tables, following Morel et al. (2002).

To operate Eqs (11) and (12) $K_d(555)$ is derived from an algorithm similar to the OK2-560 but adapted to λ =555 nm and R(555) is derived from $\rho_w(555)$ through Eq. (2).

Because Chl is needed to operate Eqs 11 and 12, this algorithm would be applied after the Chl algorithm.

It must be stressed, however, that the nominal application of such a method needs independent K_d and R estimates, which is the case when using *in situ* data. When applying the same method in the remote sensing context, the sole quantity available directly is ρ_{w} , whereas K_d is derived from a reflectance ratio (Eq. 8). It is no longer a quantity independent from R. The performance of the algorithm is, therefore, expected to be affected in this case (**this is a general statement valid for any type of IOP inversion algorithm using the remote sensing signal**).

This scheme has been tested in order to assess its performance as compared to other methods and as compared to *in situ* data. The synthetic and the *in situ* data bases previously used by the IOCCG working group on IOP algorithms (IOCCG, 2006) have been used here, as well as backscattering measurements from the BOUSSOLE site (Antoine et al., 2006), the "Plumes and Blooms" site (Kostadinov et al., 2007), and the NOMAD V2 data set (Werdell and Bailey, 2005). The results are provided in Figs. 4 to 7 below.

Figure 4 shows that the proposed algorithm is working well when applied to synthetic data.

More importantly, Figure 5 still shows good performances when the same algorithm is applied to independent *in situ* data (only for absorption). Total absorption tends to be underestimated by the algorithm; this needs to be confirmed or invalidated through additional validation exercises (using, e.g., NOMAD). It is, therefore, proposed to use Eqs 11 and 12 to derive total absorption at 443 nm.



Figure 4: Validation of the proposed IOP algorithm against the synthetic data set of IOCCG (IOCCG, 2006). The four panels are for total absorption and total backscattering at two wavelengths. The parameters of a linear regression on the log-transformed data are provided in each panel. Here K_d and R are taken from the synthetic data set so they are independent quantities

Figure 6 shows good results for the derivation of b_{bp} in the green.

It is, therefore, proposed to derive the total backscattering coefficient in the 560 nm green band. This coefficient is usually produced at 443 nm, the accuracy of which being likely affected by the presence of the large phytoplankton absorption in meso-to eutrophic Case 1 waters. In oligotrophic waters, the respective contributions of particles and seawater to the total backscattering is largely unbalanced to the advantage of seawater (the backscattering coefficient of seawater at 443 nm is 2.45 10⁻

		Ref: S3-L2-SD-03- C10-LOV-ATBD
David ANTOINE	SENTINEL-3 OPTICAL PRODUCTS AND ALGORITHM	Issue: 2.3
	DEFINITION	Date: 5 October 2012
	OLCI Level 2 Algorithm Theoretical Basis Document	Page:16
	Ocean Colour Products in case 1 waters	

 3 m⁻¹). The signal to be retrieved (b_{bp}) is therefore small and the uncertainty on its derivation is large.

These two disadvantages are largely suppressed at 560 nm. Atmospheric correction errors are also much lower in the green than they are in the blue.



Figure 5: Validation of the proposed IOP algorithm against the *in situ* data set of IOCCG (IOCCG, 2006). The four panels are for total absorption at four wavelengths (no backscattering measurements in the IOCCG data set). Here, K_d has been derived from Chl before entering into the algorithm (no K_d data within the IOCCG *in situ* data base). The parameters of a linear regression on the log-transformed data are provided in each panel. Note: data from the Chesapeake bay and its vicinity (experiment name: "LMER-TIES"), suspected of having been collected in Case 2 waters, have been removed from the data base.





Figure 6: Validation of the proposed algorithm for the particulate backscattering coefficient, against *in situ* data from the BOUSSOLE site (Antoine et al., 2006; hydroscat-II instrument), the Plumes and Blooms site (Kostadinov et al., 2007; hydroscat-VI instrument), and the NOMAD v2 data set (Werdell and Bailey, 2005; various instrument). The parameters of a linear regression on the log-transformed data are provided. The shaded area corresponds to the usual range over which inversion methods are validated, clearly showing that validation for clear waters was missing up to now.

In clear waters, getting accurate particulate backscattering coefficients, b_{bp} , requires accurate determination of the backscattering by seawater itself, b_{bw} . A recent analysis by Twardowski et al (2007) provided a refined computation for b_{bw} (used to produce the results shown in Fig. 6 here). Their recommendations should be followed, which means that the water temperature (SST) and salinity (SSS) should be known to determine b_{bw} . Sufficiently accurate climatologies exist for these two parameters so there is no need to determine their actual values to compute b_{bw} when processing OLCI data (for instance a 1psu difference in SSS for SST=20°C ends up with a 1 10⁻⁵ m⁻¹ difference in b_{bw} at 555 nm). More realistic values could be incorporated, however, and at least for SST, when reprocessing the data (e.g., weekly global products for SST such as the ones provided by the GHRSST project).

Recommendation: use the Morel et al. (2006) approach (Eqs. 11 & 12 here) to derive total absorption and total backscattering coefficients. Follow Twardowski et al. (2007)

to determine b_{bw} (to get b_{bp}) and Morel et al. (2007b) to determine a_w (to get $a_t - a_w$, i.e., the sum $a_p + a_{cdom}$). Data sources for SST and SSS to be discussed / selected during algorithm implementation.

3.1.4 Can the CDOM absorption coefficient (ag) be derivable?

The uncertainty on absorption by CDOM is known to be a major problem in the derivation of the chlorophyll concentration, for instance. An accurate determination of a_g would be, therefore, a significant advance in the retrieval of OC products in Case 1 waters. A better separation of the influence of CDOM and phytoplankton in the absorption budget is also important to improve the modelling of primary production. Deriving a_g is, however, far from easy, because the deconvolution of the effects of Chl and CDOM is largely impeded by their intermingled influences in the blue part of the e.m. spectrum. Non-algal particles also intervene.

Once the total absorption coefficient is known (see above), it is feasible in theory to decompose it into several components and the associated "partial-coefficients" corresponding to various optically-significant quantities. This is feasible by virtue of the additive character of IOPs, so that one can write:

$$a(\lambda) = a_{w}(\lambda) + a_{\phi}(\lambda) + a_{nap}(\lambda) + a_{g}(\lambda)$$
(13)

where $a_w(\lambda)$ is the absorption coefficient of sea water, $a_{\phi}(\lambda)$ is the absorption coefficient of phytoplankton, $a_{nap}(\lambda)$ is the absorption coefficient of non-algal particles, and $a_g(\lambda)$ is the absorption coefficient of coloured dissolved organic matter (also called gelbstoff, hence the "g" subscript). The sum of $a_{\phi}(\lambda)$ plus $a_{nap}(\lambda)$ is denoted $a_p(\lambda)$, standing for the absorption coefficient of all particles.

The error budget that could be derived from each component depends on the wavelength, because the relative importance of the different components is varying dramatically with wavelength.





Figure 7: Validation of the proposed a_g algorithm against the *in situ* data set of IOCCG (IOCCG, 2006). The four panels are for CDOM absorption at four wavelengths. Here, a_p has been derived from Chl following Bricaud et al. (1998). The parameters of a linear regression on the log-transformed data are provided in each panel.

Roughly speaking, it is illusory to derive $a_g(\lambda)$ with an acceptable accuracy for λ >500 nm, and it is best to derive $a_{\phi}(\lambda)$ in the vicinity of phytoplankton absorption peaks.

		Ref: S3-L2-SD-03- C10-LOV-ATBD
David ANTOINE	SENTINEL-3 OPTICAL PRODUCTS AND ALGORITHM	Issue: 2.3
	DEFINITION	Date: 5 October 2012
	OLCI Level 2 Algorithm Theoretical Basis Document	Page:20
	Ocean Colour Products in case 1 waters	

Here, the feasibility to derive $a_g(412)$ from a(412) has been examined, because (1) a_g increases exponentially in the blue, (2) water absorption is small at 412 nm, and (3) the particle absorption is not at its maximum (in other words, the relative contribution of a_g to the total absorption budget is larger). The operation to perform is:

$$a_{g}(\lambda) = a(\lambda) - [a_{w}(\lambda) + a_{p}(\lambda)]$$
(14)

The difficulty is the unavailability of a direct estimate of $a_p(\lambda)$. The use of an empirical relationship between $a_p(412)$ and Chl has been tested, following Bricaud et al. (1998). By doing so, it is assumed that the uncertainty on the Chl-derived particle absorption is still low enough for $a_g(412)$ to be derived meaningfully.

This approach has been tested on the IOCCG *in situ* data set and the results are presented in Fig. 7. An acceptable accuracy is only obtained at 412 nm. It seems, therefore, possible to derive the absorption coefficient of the coloured dissolved organic matter through this technique.

A much thorough validation is still needed, however, to definitely conclude on the appropriateness of this approach.

A data base of CDOM absorption measurements should be assembled for that purpose. It will rely in particular on data presently collected at BOUSSOLE, and on any other available data sets (e.g., NOMAD), provided that their quality is appropriate.

Recommendation: combine the total absorption, a_t , as derived from the Kd-R inversion algorithm (Morel et al., 2006: Eqs. 11 & 12 here), the Chl-derived a_p from Bricaud et al. (1998) and a_w derived as per Morel et al. (2007b) to determine $a_{cdom}(412) = a_t(412) - a_w(412) - a_p(412)$.

3.1.5 Alternative approach: the GSM algorithm

The algorithms proposed above are independent one from each other, so that the various products are separately determined from the water-leaving reflectance spectrum derived after atmospheric correction. This solution has one advantage, which is precisely to have independent estimates of each parameter, i.e., the possible error on one of them doesn't transfer as an error on the others. This solution also has some disadvantages, among which is the impossibility to derive an error estimate on each determination of the geophysical parameters. In other words, there is no possible pixel-by-pixel uncertainty estimate. The nature of these algorithms only

allows an overall uncertainty to be assessed (in general though the comparison with in situ data).

Another approach is therefore proposed here, which consists of a simultaneous determination of the inherent optical properties and derived parameters (chlorophyll via its absorption coefficient in the blue, the particulate backscattering coefficient at 443 nm, and the absorption by coloured detrital matter at 443 nm), and which is able to provide a pixel-by-pixel uncertainty estimate. This is the so-called "GSM" semianalytical algorithm (for "Garver, Siegel and Maritorena"; Garver and Siegel, 1997; Maritorena et al., 2002; Maritorena and Siegel, 2005). The inputs to this model are the spectral normalized water-leaving radiances ($L_{wN}(\lambda)$) (i.e., the full spectrum is used from 412 nm to the red).

The GSM model is briefly described below (essentially taken from IOCCG, 2006). It is based on the quadratic relationship between the remote-sensing reflectance (R_{rs}) and the absorption and backscattering coefficients (Gordon et al., 1988):

$$R_{\rm rs}(\lambda) = \frac{t^2}{n_{\rm w}^2} \sum_{i=1}^2 g_i \left(\frac{b_{\rm b}(\lambda)}{b_{\rm b}(\lambda) + a(\lambda)} \right)^i,\tag{15}$$

where g1(= 0.0949) and g2(= 0.0794) are geometrical factors. The absorption coefficient, a(λ), is decomposed into a_w(λ) (seawater), a_{ph}(λ) (phytoplankton), and a_{dg}(λ) (coloured detrital and dissolved material, CDM). Similarly b_b(λ), is partitioned into backscattering by seawater, b_{bw}(λ), and by suspended particulates, b_{bp}(λ). The non-water absorption and scattering terms are parameterized as a known shape with an unknown magnitude:

$$a_{\rm ph}(\lambda) = C a_{\rm ph}^*(\lambda),\tag{16}$$

$$a_{\rm dg}(\lambda) = a_{\rm dg}(\lambda) \exp(-S(\lambda - \lambda_0)), \tag{16'}$$

$$b_{\rm bp}(\lambda) = b_{\rm bp}(\lambda_0) \left(\frac{\lambda_0}{\lambda}\right)^{\gamma},$$
 (16'')

where $a_{ph}^*(\lambda)$ is the chlorophyll-a specific absorption coefficient, S is the spectral slope for CDM absorption (Bricaud et al., 1981, 1998), Y is the power law exponent for b_{bp} , and λ_0 is a scaling wavelength (443 nm). S, Y and $a_{ph}^*(\lambda)$ are set to constant values.

For $a_{ph}(\lambda)$, $a_{dg}(\lambda)$, and $b_{bp}(\lambda)$, the unknown magnitudes are the chlorophyll-a concentration (Chl), the detritus/gelbstoff absorption coefficient, $a_{dg}(443)$, and the particulate backscatter coefficient, $b_{bp}(443)$, respectively.

GSM validation results are shown in Fig. 8 with MERIS, SeaWiFS, and MODIS (in situ data from NOMAD data set for the 1997-2003 time period and additional data from the SeaBASS archive for the 2003-2007 period).

		Ref: S3-L2-SD-03- C10-LOV-ATBD
David ANTOINE	SENTINEL-3 OPTICAL PRODUCTS AND ALGORITHM DEFINITION	lssue: 2.3
		Date: 5 October 2012
	OLCI Level 2 Algorithm Theoretical Basis Document	Page:22
	Ocean Colour Products in case 1 waters	



Figure 8: Adapted from Fig. 11 of Maritorena et al. 2009. Matchups statistics for the three GSM merged products, Chl (left), CDM (centre) and b_{bp} (right). The colour of each matchup point indicates which satellite data sources were used for that point (green: SeaWiFS only, red: AQUA only, yellow: MERIS only, light blue: AQUA+MERIS, purple: SeaWiFS+MERIS, black: SeaWiFS+AQUA, dark blue: SeaWiFS+AQUA+MERIS).

3.2 Error estimates

3.2.1 Semi-empirical algorithm

A. Global uncertainty

For the semi-empirical algorithms proposed in section 3.1, an average uncertainty can be derived from the comparison with *in situ* data, typically providing the slope and intercept of a regression, and the associated coefficient of regression and root mean square error.

Numbers are not provided here because they depend on the database that is used for this assessment.

Such an approach can be global or regionalized to some extent (see Dowell et al., 2009).

This will have to be discussed among the Sentinel-3 group and an agreement found on which database has to be used to produce such numbers.

The reader is referred also to the MERIS ATBD 2.9 for some discussions about the uncertainties inherent to such algorithms (Morel and Antoine, 2007).

A. Pixel-per-pixel uncertainty (propagation of errors from atmospheric correction)

The uncertainties estimate proposed here is based on Taylor expansions of function of random variables. In the present case, Chlorophyll-a can be considered as a function of the two variables R1 and R2 (*i.e.*, the two reflectances used to form the "blue-to-green ratio") with input uncertainties assumed to follow Gaussian distribution of variances, and covariances $\sigma_{k_1}^2$, $\sigma_{k_2}^2$ and $\sigma_{k_1k_2}$. Then the uncertainty on Chl is given by

$$\sigma_{Chl}^{2} = \left(\frac{\partial Chl}{\partial R_{1}}, \frac{\partial Chl}{\partial R_{2}}\right) \begin{pmatrix} \sigma_{R_{2}}^{2} & \sigma_{R_{1}R_{2}} \\ \sigma_{R_{1}R_{2}} & \sigma_{R_{2}}^{2} \end{pmatrix} \begin{pmatrix} \frac{\partial Chl}{\partial R_{1}} \\ \frac{\partial Chl}{\partial R_{2}} \end{pmatrix}$$
(17)

After computing the partial derivative of Chl, one finds the general estimate

$$\sigma_{Chl}^2 = Chl^2 * \left(\sum_{i=1}^{N} A_i * i * \left(\log_{10} \frac{R_1}{R_2}\right)^{i-1}\right)^2 * \left(\frac{\sigma_{R_1}^2}{R_1^2} - 2\frac{\sigma_{R_1R_2}}{R_1R_2} + \frac{\sigma_{R_2}^2}{R_2^2}\right)$$
(18)

Where the A coefficients are those given in Table 1 (**Note:** the K_d(490) algorithm is of the same formalism than the Chl algorithm so the errors can be computed the same way for both). Assuming perfectly correlated uncertainties on R_1 and R_2 (i.e. $\sigma_{R_1R_2} = \sigma_{R_1} * \sigma_{R_2}$) minimizes the uncertainties on Chl, now given by

$$\sigma_{Chl}^2 = Chl^2 * \left(\sum_{i=1}^{N} A_i * i * \left(\log_{10} \frac{R_1}{R_2}\right)^{i-1}\right)^2 * \left(\frac{\sigma_{R_1}}{R_1} - \frac{\sigma_{R_2}}{R_2}\right)^2$$
(19)

This is illustrated on Fig. 9 for typical values or errors on he two reflectances. In the above formalism, the Chl algorithm does not propagate noise in case the relative errors in R1 and R2 and equal (which is understandable considering the band-ratio nature of this algorithm).



Figure 9: example of error calculation following Eq. (19). The errors are given on the figure.

3.2.2 GSM algorithm

Concerning the GSM algorithm, error estimates can be provided on a pixel-bypixel basis (from Maritorena et al., Remote Sensing of Environment, submitted). This paper presents the outcomes of the ESA GlobColour project to what concern error estimates based on the use of the GSM (or even GSM-like) algorithms.

For any "semi-analytical" inversion technique, a minimisation is done between a "reference spectrum model" and the observed model by iterating on values of freeparameters. The invaluable advantage is that, providing error estimates on inputs and appropriated minimisation technique, the fitting procedure provides,

		Ref: S3-L2-SD-03- C10-LOV-ATBD
David ANTOINE	SENTINEL-3 OPTICAL PRODUCTS AND ALGORITHM	Issue: 2.3
	DEFINITION	Date: 5 October 2012
	OLCI Level 2 Algorithm Theoretical Basis Document	Page:25
	Ocean Colour Products in case 1 waters	

mathematically, the range of uncertainties of inversion and, by this, the three IOP presented above, as well as their uncertainties.

This potential for providing error bars has been extensively explored during GlobColour and some consolidated results are presented below.



Figure 10: Adapted from Fig. 9 of Maritorena et al. 2009. Comparisons of the predicted and actual uncertainties using the NOMAD data set (upper left: Chl; upper right: CDM; lower left: b_{bp} . If the predicted uncertainties are accurate, about 2/3 of the data points should be below the 1:1 line. The centred variables (retrieval/error; lower right panel) show a normal distribution for CHL (circles) and b_{bp} (stars) while the CDM (triangles) distribution departs from normal (curve).

The requested qualification of inputs (as well as model uncertainties) has been done through GlobColour and propagation of error through Levenberg-Marquardt minimisation procedure has allowed production of reliable error bars at least for Chl-a and for b_{bp} . For CDM the propagation of uncertainties has proven to be less reliable and points toward a requested adaptation of the reference reflectance spectrum.

Fig. 10 shows the results for all three parameters (see the three first panels) of the retrieved error estimates wrt to actual error obtained through matchup analysis. Scatter plots for which (visually) two third of the actual error is under the 1/1 line of error estimates, indicate a satisfactory estimates of the error (as assumed to follow a normal probability function). The three normalised distribution function have been reported on the fourth panel (bottom right) and theoretically should be comparable to the normalised centred density probability function which is also sketched. Good correlation between this theoretical shape and the ones obtained for Chla and b_{bp} (while CDM deserves some attention) indicates that this approach is the one to be followed for the implementation of the OLCI L2 processing.

3.3 Summary of recommendations

3.3.1 Products

The list of products is:

- Pigment index (Chl) (OC4Me algorithm)
- K_d(490) (OK2-560 algorithm)
- b_{bp}(560) (Morel et al., 2006 algorithm)
- a_{cdom}(412) (Morel et al., 2006 algorithm)
- a_{phy}(443) (GSM algorithm)
- b_{bp}(443) (GSM algorithm)
- a_{cdm}(443) (GSM algorithm)

The marine reflectances in all visible bands ($\rho_w(\lambda)$) are obviously part of the product list as well (it is just not clear whether they are considered as the final products of the atmospheric correction, and so to be listed in the CWAC ATBD, or as the first basic ocean colour product, to be listed in this ATBD).

"Pigment index" (Chl): use the OC4Me algorithm, and include a θ_s -dependence in the \Re lookup table. Derive Chl also from the GSM algorithm (Garver and Siegel, 1997; Maritorena et al., 2002; Maritorena and Siegel, 2005).

K_d(490): use the OK2-560 algorithm (Morel et al. 2007a).

IOPs:

At λ = 560 nm only: use the Morel et al. (2006) approach (Eqs. 11 & 12 here) to derive the total backscattering coefficient (b_b). Follow Twardowski et al. (2007) to determine b_{bw} (see appendix) so that b_{bp} is obtained as b_b - b_{bw}. Data sources for SST and SSS to be discussed / selected during algorithm implementation. At λ = 412 nm only: combine the total absorption, a_t , as derived from the Kd-R inversion algorithm (Morel et al., 2006: Eqs. 11 & 12 here), the Chl-derived a_p from Bricaud et al. (1998) and a_w derived as per Morel et al. (2007b) to determine

 $a_{cdom} = a_t - a_w - a_p.$

In parallel, use the GSM (Garver and Siegel, 1997; Maritorena et al., 2002; Maritorena and Siegel, 2005) to get $a_{ph'}$, b_{bp} and $a_{cdm'}$ at λ = 443 nm.

3.3.2 Pixel-by-pixel error estimates

Semi-empirical algorithms: proceed as described in section 3.2.1 of this ATBD.

GSM algorithm: proceed as described in section 3.2.2 of this ATBD.

Acknowledgements:

Constant Mazeran (ACRI-ST) is acknowledged for his help in defining error estimates for the Chl and K_d algorithms (section 3.2.1).

4. ASSUMPTIONS AND LIMITATIONS

4.1 Assumptions

Pixel-by-pixel error estimates of the water leaving reflectance (each marine band) are available as input.

4.2 Constraints, limitations

The algorithms proposed here are valid above Case 1 waters, which means that they cannot provide reliable results when applied over Case 2 waters that would not have been identified as such (in particular turbid Case 2 waters).

The same comment is valid for any other "non-nominal" conditions of applications, including but not being limited to, coccolithophorid blooms, residual, non-identified, sun glint, non-corrected adjacency effects, cloud shadows and unidentified thin clouds.

For the chlorophyll concentration, the reader is referred more specifically to Morel (2007a) and the MERIS ATBD 2.9 for a detailed discussion of the assumptions and limitations related to the OC4Me algorithm.

For the K_d algorithm, the reader is referred more specifically to Morel et al. (2007a) for a detailed discussion about the OK2-560 algorithm.

A possible limitation of the GSM algorithm lies in the range of variability of the data bases used for its optimization. It is known that GSM isn't totally optimized for clear oceanic waters. This is under study and an improved version optimized for a larger range of trophic states is under development.

5. REFERENCES

- Antoine, D. M. Chami, H. Claustre, F. D'Ortenzio, A. Morel, G. Bécu, B. Gentili, F. Louis, J. Ras, E. Roussier, A.J. Scott, D. Tailliez, S. B. Hooker, P. Guevel, J.-F. Desté, C. Dempsey and D. Adams. 2006, BOUSSOLE : a joint CNRS-INSU, ESA, CNES and NASA Ocean Color Calibration And Validation Activity. NASA Technical memorandum N° 2006 214147, 61 pp.
- Bricaud, A., Morel, A. and L. Prieur (1981). Absorption by dissolved organic matter of the sea (yellow substance) in the UV and visible domains, Limnology and Oceanography, 26, 43-53.
- Bricaud, A., Morel, A., Babin, M., Allali, K., Claustre, H., 1998. Variations of light absorption by suspended particles with chlorophyll a concentration in oceanic (Case 1) waters: analysis and implications for bio-optical models. Journal of Geophysical Research 103, 31033–31044.
- Garver, S.A. and Siegel, D.A. (1997). Inherent optical property inversion of ocean color spectra and its biogeochemical interpretation 1. time series from the Sargasso Sea. J. Geophys. Res., 102: 18,607-18,625.
- Gordon, H.R., 1989. Can the Lambert-Beer law be applied to the diffuse attenuation coefficient of ocean water? Limnology and Oceanography 34, 1389–1409.
- Gordon, H.R. (2002). Inverse Methods in hydrologic optics. Oceanologia 44: 9-58.
- Gordon, H.R., 2005, Normalized water-leaving radiance: revisiting the influence of surface roughness, Appl. Opt. 44, 241-248.
- Gordon, H.R., Brown, O.B., Jacobs, M.M., 1975. Computed relations between inherent and apparent optical properties of a flat homogeneous ocean. Applied Optics 14, 417–427.
- Gordon H.R. and A. Morel, 1983. Remote assessment of ocean color for interpretation of satellite visible imagery. Edité par R.T. Barber, C.N.K. Mooers, M.J. Bowman and B. Zeitzschel, Lecture notes on coastal and estuarine studies, 4, 114 pp.
- IOCCG (2006). Remote Sensing of Inherent Optical Properties: Fundamentals, Tests of Algorithms, and Applications. Lee, Z.-P. (ed.), Reports of the International Ocean-Colour Coordinating Group, No. 5, IOCCG, Dartmouth, Canada.
- Kostadinov T., D.A. Siegel, S. Maritorena, and N. Guillocheau, 2007, Ocean color observations and modelling for an optically complex site: Santa barbara channel, california, USA, J. Geophys. Res., 112, C07011, doi:10.1029/2006JC003526.
- Maritorena S., D.A. Siegel & A. Peterson. 2002. Optimization of a Semi-Analytical Ocean Colour Model for Global Scale Applications. Applied Optics. 41(15): 2705-2714.
- Maritorena, S. and D.A. Siegel. 2005. Consistent Merging of Satellite Ocean Colour Data Sets Using a Bio-Optical Model. Remote Sensing of Environment, 94(4): 429-440.

- Maritorena, S., O. Hembise Fanton d'Andon, A. Mangin & D.A. Siegel. 2009. Merged Ocean Color Data Products Using a Bio-Optical Model: Characteristics, Benefits and Issues. Remote Sensing of Environment, submitted
- Morel A., 1988. Optical modeling of the upper ocean in relation to its biogenous matter content (case 1 waters). J. Geophys. Res., 93, 10749-10768.
- Morel A. and D. Antoine, 2007, MERIS ATBD 2.9, available at : http://envisat.esa.int/instruments/meris/pdf/
- Morel A., D. Antoine, and B. Gentili, 2002. Bidirectional reflectance of oceanic waters: accounting for the Raman emission and varying particle scattering phase function. Appl. Opt.41, 6239-6306
- Morel A. and B. Gentili, 1996. Diffuse reflectance of oceanic waters. III. Implication of bidirectionality for the the remote-sensing problem. App. Opt., 35, 4850-4862.
- Morel A. and B. Gentili, 2004. Radiation transport within oceanic (Case 1) waters. J. Geophys. Res., 109, C06008, doi:10.1029/2003JC002259.
- Morel, A., Gentili, B., Chami, M., and J. Ras (2006) Bio-optical properties of high chlorophyll Case 1 waters, and of yellow-substance- dominated Case 2 waters. Deep-Sea Research I, 53, 1439-1559.
- Morel, A., Huot, Y., Gentili, B., Werdell, P.J., Hooker, S.B. and B.A. Franz (2007a). Examining the consistency of products derived from various ocean color sensors in open ocean (Case 1) waters in the perspective of a multi-sensor approach. Remote Sensing of Environment, 111, 69-88.
- Morel, A., Gentili, B., Claustre, H., Babin, M., Bricaud, A., Ras, J., and F. Tieche (2007b) Optical properties of the "clearest" natural waters, Limnology and Oceanography, 52(1), 217-229
- Morel, A., and S. Maritorena (2001). Bio-optical properties of oceanic waters: A reappraisal. Journal of Geophysical research, 106, 7763-7780.
- Morel A. and L. Prieur, 1977. Analysis of variations in ocean color. Limnol. Oceanogr., 22, 709-722.
- O'Reilly J. E., S. Maritorena, B. G. Mitchell, D. A. Siegel, K. L. Carder, S. A. Garver, M. Kahru and C. R. McClain. 1998. Ocean Color Chlorophyll Algorithms for SeaWiFS. Journal of Geophysical Research, 103(C11): 24,937-24,953.
- Twardowski, M. S., Claustre, H., Freeman, S. A., Stramski, D., and Huot, Y.: Optical backscattering properties of the "clearest" natural waters, Biogeosciences, 4, 1041-1058, 2007, http://www.biogeosciences.net/4/1041/2007/.
- Wang, M. (2006), "Effects of ocean surface reflectance variation with solar elevation on normalized water-leaving radiance," Appl. Opt., 45, 4122-4128.
- Werdell, P.J., and Bailey, S.W. (2005). An improverd in-situ bio-optical data set for ocean color algorithm development and satellite data product validation. Remote Sensing of Environment, 98: 122-140.

6. Appendix: bbw computation

Computation of b_{bw} as per Twardowski et al. (2007) (Eqs. 1-3 and Table 1) and references therein:

Parameters:

k = Boltzmann constant, 1.38054 10^{-23} J K⁻¹ δ = 0.051 (depolarization ratio). SST is sea-surface temperature, in °C SSS is sea-surface salinity, in psu λ is the wavelength in nm.

Equations:

n_wat = $1.3247 + 3.3 \ 10^3 \ \lambda^{-2} - 3.2 \ 10^7 \ \lambda^{-4} - 2.5 \ 10^{-6} \ SST^2$

isothermal_compress = $(5.062271 - 0.03179 \text{ SST} + 0.000407 \text{ SST}^2) 10^{-10}$

comp1 = (-0.000156 λ + 1.5989) 10⁻¹⁰

comp2 = (1.61857 - 0.005785 SST) 10⁻¹⁰

n_pressure_derivative = (comp1 comp2) / 1.5014 10⁻¹

 $\beta_{\rm W}(90) = \frac{2 \pi^2 \text{ k (SST + 273) n wat}^2}{(\lambda 10^{-9})^4 \text{ isothermal compress}} \text{ n pressure derivative}^2 \frac{(6+6\delta)}{(6-7\delta)}$

 b_{wat} = [16 π / 3] $β_w(90)$ [(1/2) ((2+δ) / (1+δ))]

 $b_w = b_{wat} (1 + 0.3 (SSS / 37))$

 $b_{bw} = b_w / 2$

Values of b_{bw} for two bands and two SST-SSS configurations, for verification:

	$\lambda = 442 \text{ nm}$	$\lambda = 555 \text{ nm}$
SST = 20°C, SSS = 38 psu	0.004586 m ⁻¹	0.00178731 m ⁻¹
SST = 30°C, SSS = 36 psu	0.00443253 m ⁻¹	0.00172748 m ⁻¹